Physical Chemistry II (CHEM 302)
Spring 2017

Lecture: Tue, Th 10:00 - 11:15 AM, Flanner Hall 105
Discussion: We 8:15 – 9:05 AM, Flanner Hall 105
Instructor: Jan Florián

Office: Flanner Hall 314B
Office Hours: Tue 11:30 AM – 1:00 PM, We 1:30 – 3:00 PM
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Course Objectives
Part 1: Quantum Mechanics and Atomic Structure
1. Understand the basic concepts of quantum mechanics and underlying mathematics
2. Apply quantum mechanics to the study of atomic structure

Part 2: The Chemical Bond
3. Apply quantum mechanics to the study of molecular structure

Part 3: Foundations of Chemical Spectroscopy
4. Understand how light interacts with matter on the molecular level
5. Understand the relationship between quantum mechanics and spectroscopy.

Required Materials:
Physical Chemistry, Atkins & De Paula, W.H. Freeman, 10th Edition
A simple calculator (i.e. calculator not capable of being programmed or drawing graphs)

Recommended books: "*Physical Chemistry: Principles and Applications in Biological Sciences*" 5th edition, by Tinoco, Sauer, Wang, Puglisi, Harbison and Rovnyak, Pearson Education Inc. 2014, ISBN-10: 0-13-605606-7 (or previous editions)

Grade components	Maximum number of grading points
Homework	18
Exam 1	20
Exam 2	20
Final exam	42
Total	100 grading points

Homeworks: Six homework assignments, each worth of three grading points will be assigned on Thursdays. To receive full credit, a student's homework has to be submitted in person at the beginning of the next lecture. Each homework must present meaningful steps to solving assigned problems. Incorrect, late, or less than 1/3 completed homework assignments will receive zero points. Students may compare and discuss their homework solutions, but each solution has to be arrived at independently. If a students realizes during such discussion that his/her solution is likely not meaningful, he/she may attach a copy of the other student's solution along with his/her own solution and other student's name. Such augmented homeworks will receive a maximum of two grading points.

Exams: Two 50 minute mid-semester exams and one 120 minute final exam will be cumulative. No make-up exams will be administered for mid-semester exams. Students who miss a mid-semester exam for a valid reason will have the grading-point value of the final exam increased by 20 points. For the absence to be classified as having valid reason, students must notify the instructor about their absence before the exam and provide valid excuse (e.g. a doctor's note) that covers the exam day. The doctors note must be signed and contain legible name, hospital/office address and phone number and the reason for the absence. If the student disagrees with her/his score for the exam, she/he must request re-grading within one week from the day he/she received the graded exam. The exam questions may originate from end-of-chapter problems, homeworks, solved exercises from the textbook, problems solved during lecture&discussion (and their variations). Exams may also contain derivations or essays on topics presented during the lecture. Grading of all exams will include partial positive or negative credit for all significant steps taken to arrive to the final answer. Answers containing only the correct final answer without solution leading to this answer will receive 70% grading penalty. Only non-programmable scientific calculators (e.g. TI-30XA) will be allowed during exams. Students must follow the seating assignments.

Letter grades for the class will be calculated using both a fixed scale and a Gaussian scale. The scale that yields a better letter grade will determine your final letter grade.

Fixed scale
A = 100 – 80 grading points; A^- = 80 - 75; B^+ = 75 - 70; B = 70 - 65; B^- = 65 - 60; C^+= 60 - 55; C = 55 - 50; C^- = 50 - 45; D^+ = 45 - 40; D = 40 - 35; F = Less than 35 grading points.

Gaussian scale (M denotes a median value, and σ denotes standard deviation):

Earned **Grading Points**	Letter Grade	Earned **Grading Points**	Letter Grade
M – 0.2σ to M + 0.2σ	C+	M – 0.5σ to M – 0.2σ	C+
M + 0.2σ to M + 0.5σ	B-	M – 0.8σ to M – 0.5σ	C-
M + 0.5σ to M + 0.8σ	B	M – 1.1σ to M – 0.8σ	D+
M+ 0.8σ to M + 1.1σ	B+	M – 1.4σ to M – 1.1σ	D
M + 1.1σ to M + 1.4σ	A-	less than (M – 1.4σ)	F
More than (M + 1.4σ)	A		

Midterm grade: Your midterm grading points will be based on midterm exam(s) (0.7 weight) and homework (0.3 weight).

Ethical Considerations: *Students will not collaborate on any exams or quizzes. Only those materials and devices permitted by the instructor may be used to assist in examinations. Students will not represent the work of others as their own. Any student caught cheating during an exam will be reported to the Deans office and will receive zero points for the given exam.*

Class preparation: In order to understand the material presented during lectures and discussions, it is important to come to the class with good background knowledge. This can be achieved by reading (and thinking about) material in the textbook, reviewing appropriate material from calculus, physics and general chemistry classes, and solving end-of-chapter problems. Work together with your classmates; if you don't understand something, someone else may. You will also find that explaining a solution to your classmate will improve your understanding and long-term retention of the material. It is recommended that students devote to the preparation for this class a minimum of two hours every day.

Tentative Schedule

Date	Lecture topics	Reading
17-Jan	Photoelectron effect, Wave-particle duality, QM formalism I	Chapter 7A
19-Jan	Energy versus free-energy differences, Coulomb law, QM formalism II	Chapter 7B
24-Jan	Golden rule of spectroscopy, Boltzman law, QM formalism III	Chapter 7C
26-Jan	The role of models in physical chemistry, Principle of uncertainty	Chapter 7C
31-Jan	Particle in a box, Tunneling	Chapter 8A
2-Feb	QM motion in 2-D and 3-D	Chapter 8A
7-Feb	Electronic spectroscopy for the π-electron model	Chapter 8A&12A
9-Feb	**Exam 1**	review
14-Feb	Vibrational motion, Harmonic oscillator	Chapter 8B
16-Feb	Vibrations of diatomic molecules, Vibrational Spectroscopy	Chapter 8B&12D
21-Feb	Rotational motion, Angular momentum, spin, molecular rotations	Chapter 9A&12B
23-Feb	Hydrogenic atoms, Ionization energies and spectroscopic transitions	Chapter 9B
28-Feb	Many-electron atoms	Chapter 9B
2-Mar	Molecular orbital theory	Chapter 10A&B
	Spring break (March 6 – 11)	review
14-Mar	Diatomic molecules	Chapter10B
16-Mar	Polyatomic molecules	Chapter 10C
21-Mar	The Huckel approximation	Chapter 10E
23-Mar	**Exam 2**	review
28-Mar	Molecular spectroscopy	Chapter 12A
30-Mar	Vibrations of polyatomic molecules	Chapter 12D
4-Apr	IR and Raman spectroscopy	Chapter 12D
6-Apr	Electronic spectra, Beer-Lambert law	Chapter 13A
11-Apr	Fluorescence and phosphorescence	Chapter 13B

13-Apr	Magnetic resonance – general principles	Chapter 14A
18-Apr	The chemical shift	Chapter 14A
20-Apr	The NMR fine structure	Chapter 14B
25-Apr	Pulse techniques in NMR	Chapter 14C
27-Apr	EPR spectra	Chapter 14D
2-May	Final Exam, FH-105, 1-3 pm	

Notes: The instructor reserves the right to make changes to the schedule. Any changes to exam dates will be announced in class and on Sakai. Students wanting to drop lecture after midterm may stay in the co-req lab, but students with a midterm grade of F who decide to withdraw from lecture must also withdraw from the PChem lab. Students must continue to attend lecture until the week of the drop date to gain as much background knowledge as possible. Students wishing to drop lecture, and have a mid-term grade of D or better, can seek assistance from the Department of Chemistry & Biochemistry office beginning Monday March 20th at 9:00am through Monday March 27 - 4:00pm.